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Report Title

Future Directions for Selected Topics in Physics and Materials Science

ABSTRACT

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TOTAL:

Number of Papers published in non peer-reviewed journals:

(c) Presentations

Number of Presentations: 0.00

Non Peer-Reviewed Conference Proceeding publications (other than abstracts):

Received

Paper

TOTAL:

Number of Non Peer-Reviewed Conference Proceeding publications (other than abstracts):

Peer-Reviewed Conference Proceeding publications (other than abstracts):

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TOTAL:

Number of Manuscripts:

Books

Received

Paper

TOTAL:

Patents Submitted

Patents Awarded

Awards

Graduate Students

<u>NAME</u>	<u>PERCENT SUPPORTED</u>
FTE Equivalent:	
Total Number:	

Names of Post Doctorates

<u>NAME</u>	<u>PERCENT SUPPORTED</u>
FTE Equivalent:	
Total Number:	

Names of Faculty Supported

<u>NAME</u>	<u>PERCENT SUPPORTED</u>
FTE Equivalent:	
Total Number:	

Names of Under Graduate students supported

<u>NAME</u>	<u>PERCENT SUPPORTED</u>
FTE Equivalent:	
Total Number:	

Student Metrics

This section only applies to graduating undergraduates supported by this agreement in this reporting period

The number of undergraduates funded by this agreement who graduated during this period: 0.00

The number of undergraduates funded by this agreement who graduated during this period with a degree in science, mathematics, engineering, or technology fields:..... 0.00

The number of undergraduates funded by your agreement who graduated during this period and will continue to pursue a graduate or Ph.D. degree in science, mathematics, engineering, or technology fields:..... 0.00

Number of graduating undergraduates who achieved a 3.5 GPA to 4.0 (4.0 max scale): 0.00

Number of graduating undergraduates funded by a DoD funded Center of Excellence grant for Education, Research and Engineering:..... 0.00

The number of undergraduates funded by your agreement who graduated during this period and intend to work for the Department of Defense 0.00

The number of undergraduates funded by your agreement who graduated during this period and will receive scholarships or fellowships for further studies in science, mathematics, engineering or technology fields: 0.00

Names of Personnel receiving masters degrees

NAME

Total Number:

Names of personnel receiving PhDs

NAME

Total Number:

Names of other research staff

NAME

PERCENT SUPPORTED

FTE Equivalent:

Total Number:

Sub Contractors (DD882)

Inventions (DD882)

Scientific Progress

See attached.

Technology Transfer

Future Directions for Selected Topics in Physics and Materials Science

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Erin Fitzgerald –

AAAS S&T Policy Fellow in the Basic Science Office, Office of the Secretary of Defense

ABSTRACT

This report summarizes a workshop on Future Directions for Selected Topics in Physics and Materials Science that was sponsored by the Office of the Assistant Secretary of Defense for Research and Engineering, Basic Science Office. The workshop was held at the Darden School of Business on the grounds of the University of Virginia in Charlottesville, VA from January 19-21st 2011.



Summary of the Workshop on Future Directions for Selected Topics in Physics and Materials Science

Charlottesville, VA January 19-21 2011

Stu Wolf and Jiwei Lu
University of Virginia

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AAAS S&T Policy Fellow in the Basic Science Office, Office of the Secretary of
Defense

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I. EXECUTIVE SUMMARY

This report summarizes a workshop on *Future Directions for Selected Topics in Physics and Materials Science* that was sponsored by the Office of the Assistant Secretary of Defense for Research and Engineering, Basic Science Office. The workshop was held at the Darden School of Business on the grounds of the University of Virginia in Charlottesville, VA from January 19-21st 2011.

Goals: The goal of this workshop was to provide input to ASD(R&E) on emerging areas of physics with the potential for high-impact scientific breakthroughs, forming the basis for significant advances in future technologies. High-impact priorities identified over the course of the workshop are summarized in Section II.

A secondary goal was to provide a workshop assessment of how U.S. basic research stacks up to that in other areas of the world, especially in some of these areas of physics that are deemed to be of identified high leverage. This is summarized in Section III.

Participants: The workshop attendees included many university researchers and representatives from industry and national labs, a mixture of intellectual leaders in their respective fields and promising young scientists expected to be among those that will frame the directions of physics in the next few decades. The list of attendees and their affiliations is in Appendix I. In total, attendees included 25 invited scientists, five government representatives and one representative from the Australian Embassy.

Workshop Organization: The three mornings consisted of panel discussions and presentations where the invited scientists presented 10-15 minute talks focused on breakthroughs in their respective fields occurring in the last decade, followed by what they thought were the key directions for future breakthroughs in the next decade based on their expertise. After the presentations there was about an hour for the panel discussion, including a working lunch.

The first two afternoons were composed of breakout sessions followed by a reporting session. The large group was broken up into three smaller groups and asked to address several questions, the most important being what major areas had the greatest potential for advance over the next decade. On Day 1 the groups were divided by more common interests and expertise, while the second day's breakout groups were each composed of mixtures of physics sub-disciplines. After the breakout sessions on Day 1 and Day 2, the entire group re-convened for the report-out of the results of the breakouts and a group discussion.

The final day concluded with an extended discussion following the morning panel presentations, where the group integrated the recommendations of the prior two days of breakouts into a tiered list of recommended research investment priorities. The group recommended six important and generic areas for future investment,

four of a primarily scientific nature and two more directed towards enabling infrastructure development. Each of these major areas was further subdivided into more specific research topics, some of which were highlighted as being particularly important but all judged to be of notable value. Also discussed in some detail were the responses to the questions posed to all participants before and during the workshop.

Future Research Directions: The four research directions and the two infrastructure needs determined by the workshop participants to be of highest priority are listed below in no special order, and described in greater detail in Section II.

Research Directions:

- 1. New Functional Materials/Materials Discovery**
- 2. Non-Quantum Information Processing and Devices**
- 3. Quantum Information and Control**
- 4. Frontiers of Electromagnetic Science**

Enabling Infrastructure:

- 5. Experimental Tools**
- 6. Theory, Modeling and Simulation**

II. DISCUSSION OF RESEARCH DIRECTIONS AND INFRASTRUCTURE REQUIREMENTS

The workshop participants came to consensus on six major categories of recommended research priorities, four that were primarily research directions and two that were enabling infrastructure. These were further broken down into more specific directions and expanded into what might be called projects areas. Research directions considered to be the highest priorities were identified and are highlighted. This report will address each of the six major categories in turn, defining the subcategories in some detail and then describing the project level subcategories.

These categories are not orthogonal and thus may contain some overlap, but the group determined not to deliberately avoid such overlap but instead allow it to demonstrate emphasis on certain key areas. This list of research directions and infrastructure requirements is not meant to be comprehensive. They reflect the assessment of the participants with minimal input from the government organizers of the workshop.

1. NEW FUNCTIONAL MATERIALS AND MATERIALS DISCOVERY

The group felt that investment in new materials and materials discovery was very important, especially in light of the fact that many of the major materials breakthroughs of the last decade were made outside the US. Below are those areas considered to be especially interesting.

i. Materials Discovery

There are a whole host of interesting materials that have attracted significant interest starting in the last decade and which definitely are an important future direction. One type of the key and highlighted materials is that in which an order parameter (magnetic, superconducting, electronic, etc. can be controlled using an electric field. An example of such a material is a multiferroic in which there are two coupled order parameters like ferromagnetic and ferroelectric. This issue of multiferroics will come up again in the discussion of nanostructured materials, where the best multiferroics might be metamaterials. In addition to this important area, other types of materials that can have significant scientific and perhaps technological value include:

- High-temperature superconductors
- Materials that have light elements, referred to as lightides (e.g. borides, nitrides, phosphides)
- Materials for energy conversion, energy storage, energy transport and energy production:
 - Solar materials like GaN and organics or nanostructured materials that offer higher conversion efficiency
 - Magnetic materials with high energy products
 - Thermoelectric materials with enhanced figures of merit
 - Phononic materials whose phonon spectrum can be modified and controlled
- Materials for memory, e.g. magnetic, phase change, ionic etc.

ii. Motterials

Motterials are materials —mainly oxides — that have electronically-driven metal-to-insulator transitions somewhere in their phase diagram. Their electronic properties often exhibit both highly correlated and emergent behavior that depends on their structure and composition. Manganites, such as by $\text{La}_{1-x}\text{Sr}_x\text{MnO}_3$, are examples of Motterials that exhibit the aspects of strongly correlated and emergent behavior typified by their being ferromagnetic, antiferromagnetic, or paramagnetic, insulating, or conducting, depending on the temperature and the ratio of La to Sr. There are a host of other novel oxides like the vanadium oxides, the nickelates and the vanadates that may prove to be even more interesting. Very recently (not yet reported in the literature), a magnetically driven metal-to-insulating transition has been discovered in a strained thin film of calcium vanadate.

iii. Engineered and Nanostructured Materials

Highlighted by the participants was the area of engineered materials or *metamaterials*. These are materials whose behavior is not exhibited by any naturally occurring material but rather is engineered by purposeful nanostructuring. One of the more interesting metamaterials is the negative index of refraction materials that can direct and focus light in ways that natural crystals cannot. Other engineered materials that were mentioned are *superlattices* (which for example can give record thermoelectric figures of merit), *quantum dots* (for enhancing the properties of photonic structures or form plasmonic waveguides), and ordered arrays of *nanoholes* which can form photonic waveguides and resonant optical cavities. Participants also discussed the *hierarchical design of nanoscale multifunctional materials and structures* which, for example, might combine a plasmonic structure with a photonic bandgap structure in a hierarchical fashion. Finally, an area of some potential importance that is very recently emerging is the area of using *superatoms as building blocks* for engineered materials. For example certain clusters of atoms form very stable structures if the number of atoms is precisely controlled (referred to as "magic numbers"). Some of these clusters can exhibit very novel behavior, e.g. certain size clusters of aluminum and gallium are predicted to be superconducting at record high temperatures, and only recently could these clusters be fabricated; the next step would be to self organize them into macro-scale structures.

Nanostructured materials are materials whose properties depend on their having a very dimensionally constrained constituent or nanostructure. Some of the most important materials in this category are materials that are two-dimensional or exhibit 2D behavior. A key example of this type of material is *graphene*, a single monolayer of graphitic carbon. Graphene exhibits some novel electronic behaviors due to its 2D electronic structure that makes the electrons behave as massless (Dirac) particles when they are near the Fermi surface. Another example of dimensionally-constrained 2D materials is what are called *topological insulators*. These are 2D insulating materials whose top and bottom surface states are highly correlated and which can condense to form a highly conducting or even superconducting state. Finally, nanostructured materials which support the propagation and manipulation of surface plasmons may open up new structures in optics and electronics which are frequency agile and thus are "tuneable."

iv. Hybrid Systems

The *hybrid systems* category of new materials is based on the observation that when materials are combined for new functionality, the interface between these different materials is crucial and in fact can dominate the properties. The various interfaces that need to be explored for this important emerging area include the interfaces between organic and inorganic materials, the interfaces between various biomaterials, the interfaces between soft and hard materials, and the interface between various oxides. In fact, some very recent work has demonstrated that, due to strain and oxygen vacancies at the interface between two different oxides, the

properties of the interface can be drastically modified. For example, the interface between two dissimilar but insulating oxides can be metallic, magnetic or even superconducting. Finally, there is interest in the physics community in defining a strategy for multilayer combinatorics which will provide even more new functionality as additional and different types of materials, and their respective interface effects, are added.

2. NON-QUANTUM INFORMATION PROCESSING AND DEVICES

Research efforts in the area of non-quantum information processing and devices were considered to be quite important by all participants and reflect widespread interest in the future of electronics “beyond CMOS.” There is a lot of interesting science in this area, generally taking place very close to technology since the semiconductor industry considers the area essential for future technical advances. A couple of key areas were identified, and to some extent these were a key contribution of the workshop’s industrial participants.

One key area was the development of *oxide nanoelectronics*. The very basic electronic and ionic properties of various oxides were viewed as one pathway to future information processing technology. Of course, finding a *new state variable* to replace or complement charge is another key potential research direction with candidate variables including spin and phase change. Other novel topics that emerged in the course of workshop are as follows:

- *Hybrid functional systems* for combining sensing, computation and communications
- Controlled chaos for communication
- Morphable logic and electronics
- 3D and multistate integration and storage
- Bio-inspired computation and information processing
 - Neural network architectures and devices
- Distributed nanosystems and sensors
- Silicon photonics

3. QUANTUM INFORMATION AND CONTROL

The primary research direction of a number of participants is in the area of quantum information control. This area is often considered to have attracted some of the best physicists of this generation and also has attracted many top students because of its very fundamental nature as well as its technological potential. Three important directions were determined to be of significant interest for future funding and developments.

- **Development of Quantum Information Theory:** This mainly refers to the development of new algorithms that provide a significant advancement in capability over their classical equivalents. The explosion of quantum information science was precipitated by the development of Shor's factoring algorithm and Grover's search algorithm in the mid 1990s, offering quantum solutions to classically intractable problems. There is optimism that quantum information theory will provide new and even more exciting algorithms in the future.
- **Applications of Small-scale Controlled Quantum Systems:** The "holy grail" of quantum information research is the development of a full scale and scalable quantum computer. However, similarly impactful is the development of small scale quantum systems that can perform very interesting science and can and will lead to some very novel technology. Some of these are:
 - **Quantum Simulation of Quantum Systems** is using one quantum system (e.g., atoms trapped in an optical lattice) to simulate other quantum systems that are difficult or nearly impossible to simulate using classical computers
 - **Quantum Metrology** is using entanglement of quantum states for sensors and clocks. This has already led to the development of the world's most accurate clocks and some novel magnetic sensors
 - **Quantum Networks** use superposition and entanglement of a few qubits to provide long distance secure optical communication or key distribution using a quantum repeater (the simplest quantum computer).
 - **Control and Manipulation of Single/Multiple Quanta** use various resonance techniques to precisely control the quantum state of single or a few quanta. Magnetic Resonance Force Microscopy, or MRFM, has already demonstrated the observation and control of single or a few spin quanta.

In addition to these described areas the workshop participants suggested that there would be a significant benefit to exploring how to better interface the atomic, molecular and optical (AMO) techniques for qubit control with Condensed Matter approaches (currently based on spin qubits or superconducting Josephson Junction qubits).

Another area highlighted for investment is research on classical methods of controlling quantum systems, as well as the exploration of finite quantum systems like clusters and superatoms.

4. FRONTIERS OF ELECTROMAGNETIC SCIENCE

The last decade has seen many new advances in electromagnetic science. The two research aims that were considered by the participants to be the most important directions ahead in this area were as follows:

- **Precision Control of Electromagnetic (EM) Fields:** The discovery that short laser pulses produce very precise frequency combs (Nobel Prize in 2005) has opened the door to a remarkable host of science and technology and enables precision spectroscopy into the deep UV and enhanced stability of optical clocks. The discovery of structures exhibiting a negative index of refraction (metamaterials) also has the potential of evolving into many new ways of controlling, focusing, and directing photons. Finally it was only very recently realized that disordered media (opaque) could be utilized to control the propagation of light, particularly the fact that even after multiple scattering events the light remains coherent with high information content! Thus new random media lasers are now possible, and this relaxes many requirements on laser media and opens the door to very novel lasers.
- **Novel Micro and Nano-photonic and Electronic Devices:** A number of new directions based on novel materials and structures were discussed under this heading and they are listed here
 - *Tunable dielectrics.* This refers to the ability of certain materials (paraelectrics) to have a dielectric constant that is a function of the electric field applied. This would be quite important for all kinds of agile electronics. A key direction is finding ways to reduce the dielectric losses in these materials or structures.
 - *Plasmonic nanostructures.* Metallic dots or other highly conducting nanostructures can be very effectively coupled to photonic fields so that the “light” propagates as a plasma wave (a collective excitation of the electrons) in the highly conducting structure, but since the “light” propagates at the Fermi velocity rather than c , the velocity of light, we get *x-ray wavelengths at optical frequencies*. So that coupling the “light” to other electronic nanostructures doesn’t have a large size mismatch.
 - *Photonic Bandgap Materials.* In this case an ordered array of holes in a thin dielectric film with ordered defects (no hole) can be used to direct and trap light and can be used as both optical waveguides and cavities. The more precise the location and shape of the holes, the lower the loss.

Some other directions were identified and although these were not highlighted by the participants, they may prove very important in the coming decade.

- **Attosecond/High Electric Field Physics:** It has recently been possible to construct pulsed lasers with attosecond long pulses and extremely high

electric fields generated during the pulse. This opens up the door to look at material and device properties in unprecedented ways and in regimes of electric fields unobtainable until recently. It also opens up very interesting ways of optical beam combining.

- **Mm-wave/THz Technology:** It is becoming much easier to produce EM photons in this frequency range and the ability of exploiting these frequencies for spectroscopy and other important studies is becoming possible in a much wider arena.

We now will discuss the other two very major physics directions that relate to and support the four directions that have already been discussed, and point to a need for the development of infrastructure.

5. EXPERIMENTAL TOOLS

One of the strongest takeaways from the workshop discussion on high priority research investments to advance physics was not a new field at all, and will be expanded upon further in the questionnaire section (Section III) of this summary document: Namely, **researchers are no longer able to procure many essential known materials of very high quality that are “made in the U.S.A.”** In particular the issue of oxide substrates for the growth of thin films of new or emerging materials and structures was discussed in detail; at the current time, these substrates can only be procured from Europe or Asia as there are no domestic sources. This is a crucial need, not only for physical science discoveries but for our national security. We cannot stay at the forefront of technology without having control of an essential major resource. This also applies to high quality single crystals of materials needed for other important studies. For example the best low-defect diamond films come from Japan, and these are key to the development of spin qubits for the quantum information programs as described in Subsection 3.

Beyond this essential infrastructure need, the tools that were identified as important for the future of the directions that were discussed above are described below, the most important in bold font:

- **Tools for the control and characterization of interfaces of emerging/novel/meta-materials at the atomic scale:** knowing where all the atoms and spins are, knowing the oxidation states, the bonding etc.
- Nanoscale characterization
 - Dynamic 3D nanoscale imaging
- Functional Molecular spectroscopy systems
 - Nano MRI
 - Chemical and Biological sensing
- Remote tomographic imaging

The workshop participants felt that to maintain scientific progress in important fields of physics, these tools should be readily available — if not at individual institutions, then at minimum in regional centers that are within driving distance of the major academic institutions needing to use them.

6. THEORY/MODELING/SIMULATION

These recommendations for developing important theoretical tools were felt to be part of an important infrastructure for a complete understanding of many of the materials and structures mentioned above. One important point emphasized at the workshop was that most important ab-initio codes for electronic structure calculations — the starting point for many theoretical investigations of new materials or compounds — have been developed in Europe and not in the US. Apparently it is not viewed as important to the funding agencies to take the theoretical ideas pioneered in the US (e.g., by Nobel Prize for Walter Kohn) and turn them into homegrown useful codes for the community at large.

Also included in this category are some of the mathematical techniques that were originally “orphans” from other categories but were integrated in this more general area (identified below in *italics*):

- Numerical simulations
 - Ab-initio, modular tools for the entire periodic table
 - Classical simulations of quantum systems
 - Materials-by-Design: determine the material with given properties, i.e. superconducting , magnetic etc
- Mathematics of multi-scale systems
 - Interactions of stochastic modeling/design and large scale computation
 - Non-equilibrium properties
- *Compressed sensing*: This is potentially a game changing technique for the analysis of spectroscopic data where the data is sparse, yielding significant speedup in analysis.
- *Noise Analysis*: Understanding and minimizing the impact of noise e.g. stochastic resonance.

III. OBSERVATIONS FROM THE BREAKOUT DISCUSSIONS

The complete breakout session summaries will be provided as an Appendix to this report (Appendix II). However, in this section we will provide some more subjective discussion of some of the key conclusions of these breakout sessions with a brief discussion of some of the questions that were posed.

Question 1. What have been the major breakthroughs in your field during the last decade?

The breakout summaries (Appendix II) provide the lists (which are quite long and comprehensive), but the key answers have been discussed within Section II.

Question 2. What new areas do you see emerging in the next decade?

The breakout summaries and Section II are a very good summary of what have been identified as the important emerging areas in the next decade, and in fact compose the crux of this report.

Question 3. Where are the Centers of Excellence? Where do you think the best work will be done? Are they in the US?

Of course this question can be answered differently depending on the specific area of physics research. However, in general it was noted that the center of mass of many of the areas has been moving out of the US, and in other areas the US is not dominant at all. In still other areas US research remains competitive or in the lead, but clearly the US is not the dominant scientific powerhouse it once was.

One of the more concerning facts that emerged in the course of workshop discussion was in the area of research infrastructure (see also Section II, Subsection 4). The US no longer has the capacity for making or growing the highest quality crystals, substrates or other key materials; its industrial sector doesn't make the best tools for fabricating and characterizing materials and structures; and US researchers are not writing the user friendly codes for *ab-initio* theoretical modeling. It was the fully concurred recommendation of the workshop participants that there needs to be a concerted and directed effort to rectify these issues!

Question 4. What areas do you think need continuing or expanded support?

This question is subsumed in the prior section but again the full breakout summaries are attached.

Question 5. Are there particular infrastructure needs that the DOD should be investing in?

This is covered in Section II.

Question 8. Most important, what are the five most important directions that have to be supported in the next decade?

This is the basis for Section II and the workshop participants did reach a reasonable consensus on the most important directions to be pursued in the area of Physics and the related Materials Science.

IV. CONCLUSIONS

This workshop was a learning experience that for the most part accomplished the goal of determining some important areas that are judged to be high leverage investments. The agenda and process used in this workshop is not intended to be a top-down recommendation or roadmap to various agencies and program managers to direct their programs. Rather, the findings and recommendations which have come from these discussions are considered to be a strong indicator of the potential of some areas of physics and the related aspects of materials science that are new, exciting and hold strong promise for the future. While there is no claim that this list of priorities is comprehensive, the fact that there are so many areas of scientific opportunity to be exploited bodes well for the future of discoveries within the disciplines of physics, materials science and electrical engineering.

Appendix I: List of Workshop Attendees

Bill Butler, UAL & ORNL	Mikhail Lukin Harvard	Darrell Schlom Cornell
Peter Delfyett UCF	Mark Lundstrom Purdue	Ivan Schuller UCSD
Erin Fitzgerald OSD ATL	Olivier Pfister UVA	Michael Shlesinger ONR
William J. Gallagher IBM	Warren Pickett UC Davis	Robin Staffin OSD ATL
Peter Gerhardy Australian Embassy	Gernot Pomrenke AFOSR	Mircea Stan UVA
Avik Ghosh, UVA	Joe Poon UVA	Susanne Stemmer UCSB
Philip Kim Columbia	Trey Porto NIST & UM	Andy Wiener Purdue
Vitaly Kresin USC	John T. Prater ARL/ARO	R. Stanley Williams HP
Jean Pierre LeBurton UIUC	Dan Ralph Cornell	David Wineland NIST Boulder
Jeremy Levy UPITT	Stephen Russek NIST	Stu Wolf UVA
Jiwei Lu UVA	Leonid Ryzhik Stanford	Beth Beal UVA

Appendix II: Panels and Reports of Break-out Sessions

Jan 19th (Day 1) – Focused

Group I

1. Philip Kim
2. Jeremy Levy
3. Warren Pickett
4. Joe Poon
5. Darrell Schlom
6. Ivan Schuller
7. Susanne Stemmer
8. Dan Ralph
9. Steve Russek

Group II

1. Avik Ghosh
2. Jean Pierre LeBurton
3. Mark Lundstrom
4. Mircea Stan
5. Peter Delfyett
6. Stan Williams
7. Vitaly Kresin
8. Bill Butler

Group III

1. Mikhail Lukin
2. Trey Porto
3. David Wineland
4. Bill Gallagher
5. Olivier Pfister
6. Leonid Ryzhik

Jan 20th (Day 2) – Mixed

Group I

1. Joe Poon
2. Susanne Stemmer
3. Avik Ghosh
4. Mircea Stan
5. Vitaly Kresin
6. Mikhail Lukin
7. Bill Gallagher

Group II

1. Jeremy Levy
2. Darrell Schlom
3. Dan Ralph
4. Jean Pierre LeBurton
5. Peter Delfyett
6. Bill Butler
7. Trey Porto
8. Olivier Pfister

Group III

1. Warren Pickett
2. Ivan Schuller
3. Steve Russek
4. Mark Lundstrom
5. Stan Williams
6. Andrew Weiner
7. David Wineland
8. Leonid Ryzhik

Report 1: Group I, Day 1

1. Major Breakthroughs

- Nanostructured materials with New Physics (thermoelectrics,
- Fe based superconductors
- Graphene
- Topological Insulators
- Complex Oxide Heterostructures
- Multifunctional Materials
- Control and synchronization of Chaos
- Spintronics
- 3D Nanoscale characterization
- Quantum control/computing
- Realistic computer simulations

2. Emerging Areas Next Decade

- Biophysics
- 3D and Multistate Integration
- Dynamical Atomic Scale Imaging
- Systems and control with/of emergent behavior
- Design of nanoscaled multifunctional materials
- Ab-Initio modular simulation for entire periodic table
- Beyond CMOS-new state materials, nanoelectronics
- Controllable chaos, Programmable Devices (Morphable logic & electronics)
- New approaches to energy conversion and storage
- Higher T_c superconductors

3. Centers of Excellence

- Nonlinear science (60% non US)
- Novel Materials

4. What areas to expand

- Same as 2

5. New Infrastructures

- Major equipment (~ \$ 1M, > DURIP,
- Operation funding
- Agreements with large facilities
- Lithography
- Table top synchrotrons
- High resolution EM
- Crystal growth

6. Division of Funding

- Long range
- Disruptive research

8. Most Important Directions

- New Materials Discovery
 - Higher T_c superconductors
 - Design of nanoscaled multifunctional materials
 - Emergent Behavior
 - Energy conversion and storage
- Novel Devices
 - Beyond CMOS-new state materials, nanoelectronics
 - Controllable chaos, Programmable (Morphable logic & electronics)
 - 3D and Multistate Integration and storage
- Numerical Simulation
 - Ab-Initio, modular for entire periodic table
 - Multiscale
 - Quantum simulations
- Nanoscale characterization
 - Dynamic.3D nanoscale imaging
- Biophysics and Soft Matter
 - Detectors
 - Remote tomographic imaging
 - Interfaces with other soft an hard materials

Report 2: Group II, Day 1

1. What have been the major breakthroughs in your field in the last decade?

- New materials:
 - C-materials (CNTs, graphene)
 - Correlated solids/oxides
 - Metamaterials
 - Superatoms/nanodroplets
 - Highly spin polarized materials
- New paradigms:
 - Ability to engineer metamaterials for phonon/plasmon/photon/charge/spin flow
 - Optical frequency combs for very precise periodicity
 - Continuing to push Moore's law (projected to 8 nm currently)
 - Beyond Moore, entirely new kinds of switching demoed (tunnelFETs/NEMFETs)
 - New ways to drive a bit (e.g. rotating magnets with strain/current)
 - Ability to manipulate single quantum objects (e.g. detecting single dangling bond)
 - NVRAMs/Memristors
- New instrumentation:
 - Deep sub-lambda Lithography
- New computational accomplishments:
 - Finite Difference Time Domain for nano-photonics
 - New hybrid functionals (B3LYP/B3PW91 etc) for DFT bandstructures, advances in GW
 - Combining quick empirical with rigorous techniques: DFT-tight binding, Extended Huckel for bandstructures, ..

2. What new areas do you see emerging in the next decade?

- Material:
 - Correlated systems/condensates
 - C-nanoelectronics
 - biomimetics/bio-compatible and bio-inspired electronics
 - metamaterials/atomically engineered materials, Complex bio-molecules/clusters
- System Level Issues:
 - 3D hybrid integration/photronics-CMOS
 - Intelligence/Human Computer interactions
- Devices:
 - Low power electronics/spintronics (novel switches)
 - Phononics
- Algorithmic:
 - Non-Boolean/analog computing using oxides

- Metrology:
 - Noise -- metrology and as characterization tool
 - Integrated freq combs locked to BECs
- Computational:
 - Nonequilibrium correlated systems and multiscaling transport (Formalism and Computation)
 - Multiscaling electronics/spintronics
- Architecture Design:
 - Hierarchical design (atoms to circuits)

3. Centers of Excellence

- International:
 - Lot of effort in China (Academia Sinica)
 - Certain classes of effort (e.g. computational infrastructure development for electronic structures) primarily Euro-centric
- Industrial:
 - Samsung
- Labs:
 - NIST

4. Areas for expanded or continued support

- Materials:
 - Carbon
 - atomically engineered structures
 - also conventional materials (eg III-V)
 - metamaterials for thermoelectrics/phononics etc
- Device:
 - Low-power electronics/spintronics
 - Phononics (engineering energy flow)
 - bio-inspired computing
 - correlation driven switches (MITs)
- Formal/Computational:
 - Understanding nonequilibrium correlations Multiscaling of nonequilibrium properties
- Infrastructural:
 - "Virtual robots"/Avatars for back-end work, perhaps integrated with Intelligent front-end work
- Algo:
 - Non-Boolean for front end computing/signal processing

5. Infrastructure Needs

- Possibility of a centralized, consolidated fab (like Sandia/Albany but open to research community)

- Analogous model for computational resources investment in parallelizing scientific codes
- How do you feel about the current way DOD funds are apportioned between very basic, directed basic and mission oriented basic research?
- Perceived change from more basic to device centric research
- Pointed to Academia Sinica/Early day Bell Labs (scope for serendipitous Discovery)

6. Most importantly (and we will work towards a consensus on this) what are the five most important directions that need to be supported in the next decade? Each breakout will come up with 5.

- Electronics/Photonics/Magnetics/Phononics
- Computation: Emerging (e.g. nonequilibrium properties) vs. existing but expanded (refined bandstructures etc)
- Utilizing correlated systems
- Connections to Biology (perception: Many interdisciplinary issues, e.g. bio-inspired electronics, falls through cracks with NSF/NIH)
- Novel Materials/Novel variables for info processing (Beyond Moore)

Report 3: Group III, Day 1

1. Major breakthroughs

- Quantum control
 - Demonstration of Divencenzo criteria for quantum information processing
 - Move towards scalability
 - 1) 2-D JJ surface architectures
 - 2) 2-D atomic arrays
 - Significant advances in JJ's and circuit QED
 - Simulation: first steps in atomic systems applied to many-body correlations
 - Optical waveguide systems
 - Quantum memory, light-matter interface, networks
 - Atom-like systems
 - Nanomechanics
 - Quantum nano-photonics
- Metrology
 - Optical clocks (inaccuracy $< 10^{-17}$)
 - Site-specific magnetrometry
 - Atom interferometry
 - Spectroscopy with combs
 - Use of quantum logic and entanglement
- Ultra-cold physics
 - Cold molecules
 - Fermions
 - Correlated systems
- Applications
 - Tests of fundamental physics
 - 1) quantumness of macroscopic systems (e.g., Leggett et al.)
 - 2) scaling up entangled systems
- Short-pulse; high intensity lasers
 - Snapshots of electron dynamics
- Applied mathematics
 - Compressed sensing
 - New computational tools (e.g., matrix product states)

2. Emerging fields

- Quantum control
 - Larger, more complex manipulations
 - 1) need better classical control, methods to scale
 - Quantum repeaters and networks

- New quantum systems
 - 1) topological systems
 - 2) room-temperature condensed matter systems
 - Simulation
 - 1) goal: discover some new physics or perform useful simulation better than with classical method
 - Hybrid quantum systems (e.g., atomic memory for SC qubits, nano-mechanical quantum transducers)
 - Quantum nano-photonics
 - Metrology
 - Geodesy (clocks)
 - Quantum-enhanced measurement (entanglement-enhanced sensitivity)
 - Micro/nano MRI
 - New quantum sensors
 - Applied mathematics
 - Application of compressed sensing
 - Uncertainty quantification
 - Multiple-scale systems
3. Centers of Excellence (with apologies...)
- Abroad
 - Max Planck
 - Innsbruck
 - ETH (Zurich)
 - Tokyo
 - Paris
 - Emerging centers (substantial funding)
 - 1) Singapore
 - 2) ICFO (Barcelona)
 - 3) Australia
 - 4) Waterloo
 - US
 - NSF Frontier centers
 - 1) JILA
 - 2) CUA (Harvard/MIT)
 - 3) JQI (U.Md./NIST)
 - NIST
 - Applied Mathematics
 - 1) NYU

- 2) Stanford
- 3) UCLA
- 4. Expansion/continuation
 - See items in 2)
- 5. Infrastructure needs
 - Materials improvement development for quantum science
 - Optics: sources, detectors ...
 - China current leading source of new optical crystals
- 6. DOD funds apportionment
 - Danger of focusing primarily on milestone-driven, short-term research
 - Basic research requires long-term strategy and programs
 - Need more curiosity-driven research (e.g., first 50 years of ONR basic research program)
- 7. Five Important directions
 - Quantum information theory (e.g., new algorithms)
 - Scientific interface between AMO and condensed-matter (e.g., hybrid systems)
 - Quantum science and engineering (e.g., improved classical control of quantum systems, materials research)
 - Applications of small-scale controlled quantum systems (e.g., quantum sensors, simulation, networks, integrated photonic circuits, clocks)
 - Mathematics of multiple-scale systems (e.g., interaction of stochastic modeling and large scale computation)

Report 4: Group I, Day 2

1. Major Breakthroughs

- GaN: crystal growth/non-polar orientation.
- Novel Lithography: nano-imprinting/dip-pen/self-assembly/roll to roll printing.
- NV center in Diamond.
- Atomic vapor magnetometer.
- Nano-instrumentation.
 - Macromolecule beam diffraction.
 - Aberration-corrected TEM.
 - Local structure x-ray diffraction.
 - Chip level plasmonics.
 - Free electron laser for microstructure analysis.
 - Surface enhanced Raman (single molecule detection).

2. Emerging Areas Next Decade

- Phononics
 - Nanostructured thermoelectrics
- Random laser
- New solar materials:
 - GaN, Organics,
 - Nanostructured materials (Superlattice, QD, nanoparticles, tri-metasphere (TMS)),
- THz and millimeter wave:
 - Sources
 - Transmitter
 - Detectors
- THz speed electronics: Transistors.
- MW circuitry/devices.
- Beyond 60 mV/dec sub-threshold switch (Beyond CMOS)
- Strongly correlated systems.
- Skyrmion

3. Centers of Excellence

- Phononics
 - US
- Photonics
 - Europe
- Random laser
 - ?
- New solar materials.
 - US
 - Germany
- THz and millimeter wave/THz speed electronics: Transistors.

- US
- UK
- Germany
- MW circuitry/devices.
 - US
- Beyond 60 mV/dec sub-threshold switch (Beyond CMOS)
 - US
- Strongly correlated systems.
 - Japan
 - Europe
 - US
- Skyrmion
 - Japan
 - Germany

5. New Infrastructures

- Crystal growth:
 - Non-linear optics...
 - GaN substrate
- High purity rare earth sources
- Liquid Helium
- Funds for mid-size equipments (\$ 0.5~1 Mil.)

8. Most Important Directions

- Finite Quantum system/clusters/superatoms/Droplets.
- Non-linear phenomena and complexity
 - Random laser
 - Neuro-science
 - Noise...
- Microwave/THz technology
- Frequency/Laser combs
- New solar materials:
 - GaN, Organics,
 - Nanostructured materials (Superlattice, QD, nanoparticles, tri-metasphere (TMS)),

Report 5: Group II, Day 2

1. Breakthroughs

- Measurement tools
 - Aberration correction microscopy
 - photoemission microscopy
 - spectroscopic STM
 - X-ray microscopy, etc.
- Attosecond / High Field Physics
- Integrated Optics – for Quantum Information, for increased functionality, chip scale systems
- Ceramic laser host materials
- Laser beam combining

2. Emerging Areas

- Oxide-Nanoelectronics/Ionics – e.g., electron/ion dynamics at the nanoscale

4. Areas of Expanded/Continuing Support

- Control and characterization of interfaces of emerging/novel/meta-materials at the atomic scale
- Improving (reducing) the size/cost/efficiency/of state of the art components/devices/ tools, e.g., frequency combs → reducing cost of enabling tools can be transformative.
- Strain control of nano-engineered materials (could this be done in bulk...?)
- Electrical control of order parameters (e.g., spin, superconductivity, metal insulator transitions, polarization, etc...)

5. Infrastructure

- Need fab capabilities (optical) that can meet metrics for quantum information e.g., waveguide loss, etc
- Crystal growth – nonlinear crystals, laser host materials (ceramics), correlated electron materials

6. Apportioning of DoD Funds

- Decision between basic research/mission oriented Is this a good way to ask the question...?
- Mission oriented should allow for more exploratory research.
- Should funding follow what's fashionable?
- Should funding be related to past performance?
- Should the size / length of awards be increased? (1 proposal per student - PhD?)
Need to have continuity

- More MURIs...?

7. Barriers

- Need 3D probes that can go through material that selectively interacts or interacts weakly
- DoD Solution → Initiate MURI's in these areas
- Lack of interface control on new meta-materials

8. Most Important Directions

- Electrical control of order parameters (e.g., magnetic properties, spin, superconductivity, metal insulator transitions, polarization, etc...)
- Manipulation of single/multiple quanta
- Control and characterization of interfaces of emerging/ novel/ meta-materials at the atomic scale (e.g., knowing where all the atoms, spins, oxidation states, etc., are)
- Attosecond/High Field Physics (new materials, e.g., ceramics, new source approaches, e.g. beam combining, ...)
- Oxide-Nanoelectronics/Ionics – e.g., electron/ion dynamics at the nanoscale

Report 6: Group III, Day 2

1. Major breakthroughs

- Frequency combs and metrology
 - Control subwavelength EM
 - Control time and spatial degrees of freedom
 - Near field imaging
 - Artificially structured nano-matdevice (metamaterials, Mottearials, thermoelectrics)
 - nanorandom
 - Single molecule spectroscopy without marker
 - Short time scale dynamics (atto second, pump-probe)
 - Quantum information exchange (JJ, MEMS,

2. Emerging Areas Next Decade

- Functional Molecular spectroscopy
- 3D and Multistate electronics
- Hybrid systems (materials, devices, functions)
- Distributed nanosystems and sensors
- Strategy for multilayered combinatorics
- Lightides (borides, nitrides, phosphides,
- New applications for frequency combs
- Energy conversion, production & storage (e.g. beating the Queisser-Shockley limit)

3. Centers of Excellence

- Novel materials discovery (US very low)
- Biomaterials (US leading, NIH funding [?])
- Characterization (US 50%)
- Fab lines and materials processing (US low)
- Solar cell production (US #4)
- Quantum computation (30%)

4. What areas to expand

5. New Infrastructures

- Lack of domestic suppliers of high end substrates, equipment,
- New educational opportunities – scholarships
- Industrial labs

6. Division of Funding

- Long range
- Disruptive research

7. What would be a proper division of 6.1?

- Keep all for long term-“basic”
- Reverse mission creep
- Metric base?
- US must become an innovation machine

8. Most Important Directions

- Functional Molecular spectroscopy system
 - Nano MRI
 - Chem and Bio sensors
- Novel electronics and systems
 - 3D and Multistate electronics
 - Distributed nanosystems and sensors
 - Hybrid functional systems (sensing, computing, communicating)
- New Materials
 - Strategy for multilayered combinatorics
 - Lightides (borides, nitrides, phosphides)
- Energy conversion, storage and production
- Precision control of EM fields
 - New frequency combs & applications
 - Controlled propagation in disordered media/sub-wavelength